

Learning to Branch

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Slides: www.pgupta.info/talks

To **improve** the extent to which neural networks can **imitate** a *computationally expensive but accurate heuristic* to solve mixed-integer linear programming (MILP) problems.

Outline

Problem formulation

Hybrid Models for Learning to Branch
(NeurIPS 2020)

Lookback for Learning to Branch
(TMLR 2022)

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- Discrete Optimization
- Branch-and-Bound
- The Branching Problem
- Learning to branch

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Mixed-Integer Linear Program (MILP)

$$\arg \min_x \quad c^\top x$$

- ▶ $c \in \mathbb{R}^n$ the objective coefficients

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NP-hard problem.

Applications

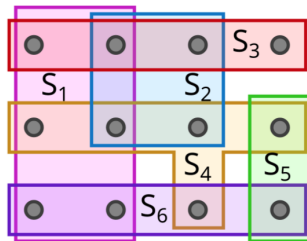
Combinatorial Auctions

Facility location-Allocation

Maximum Independent Set

Set Covering

and many more ...



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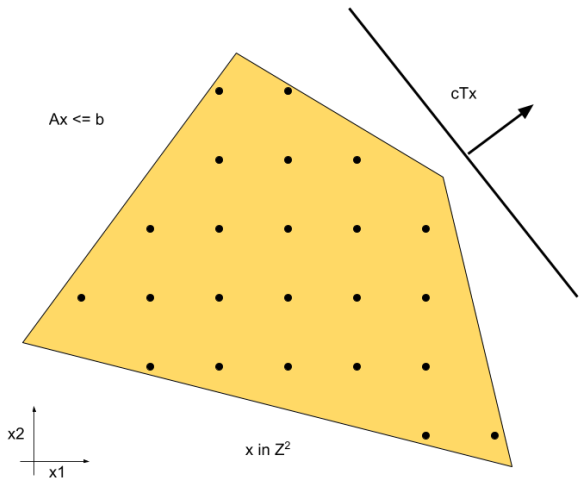


Image credit: Maxime Gasse

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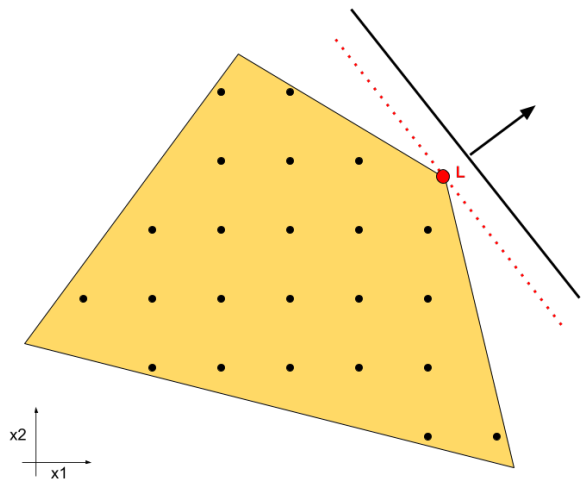
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- Polynomially solvable
 - Yields lower bounds to the original MILP

LP Relaxation of a MILP



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Branch-and-Bound (B&B)

B&B (Land et al., 1960) is the widely used framework to solve MILPs.

It consists of two steps



Each node in branch-and-bound is a new MIP

Image source: <https://www.gurobi.com/resource/mip-basics/>

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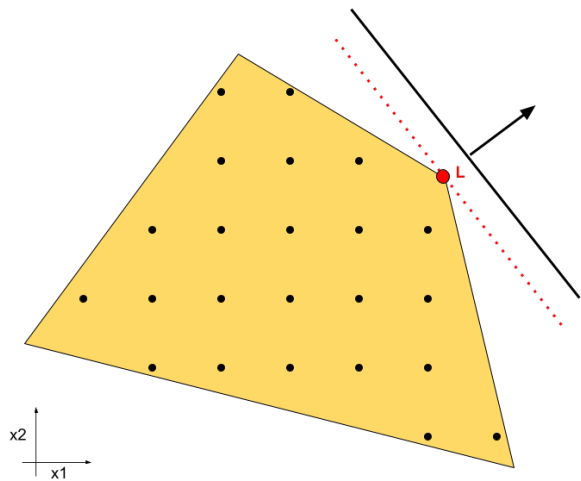
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- ▶ **Branching** - Select variable to split the problem into two
- ▶ **Bounding** - Solve the LP relaxation of resulting problem to obtain optimization guarantees on the solution

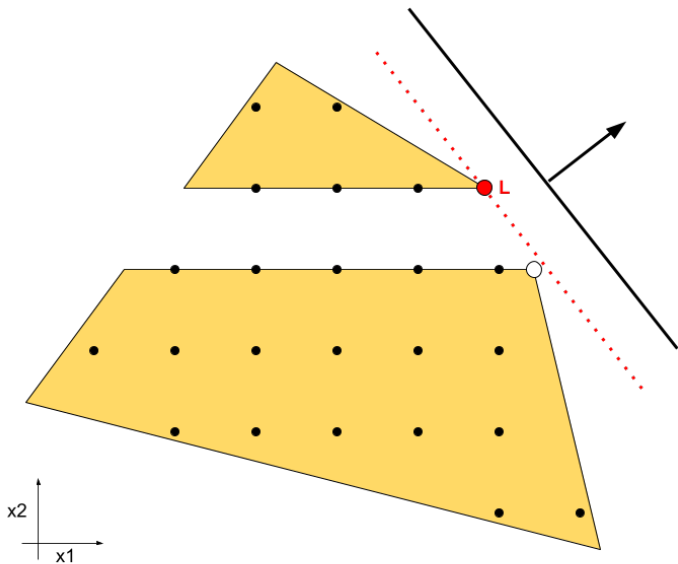
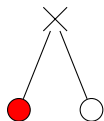


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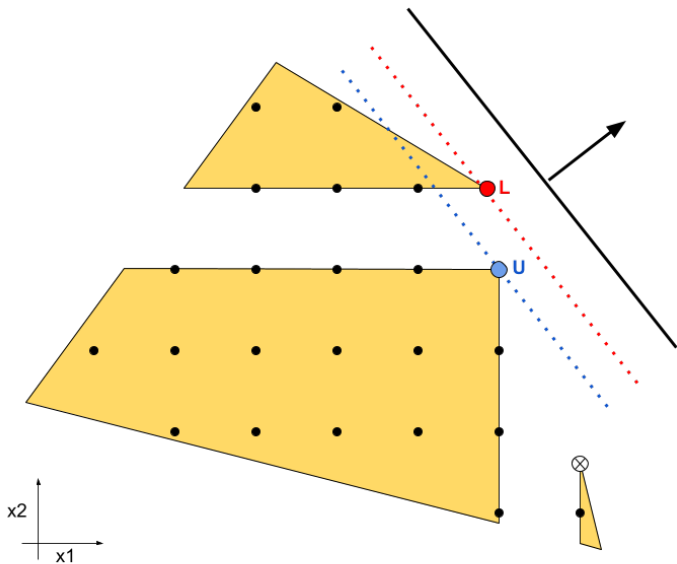
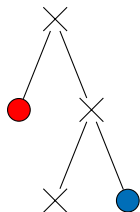
LP Relaxation of a MILP



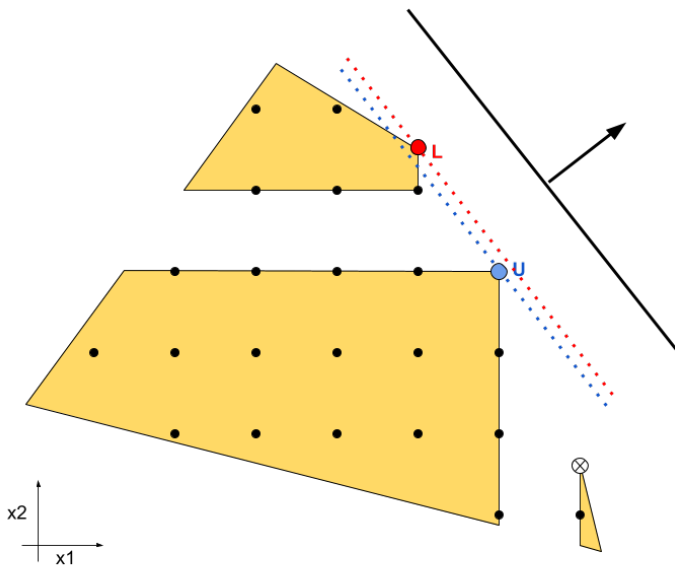
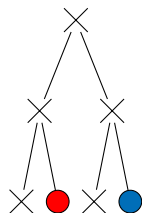
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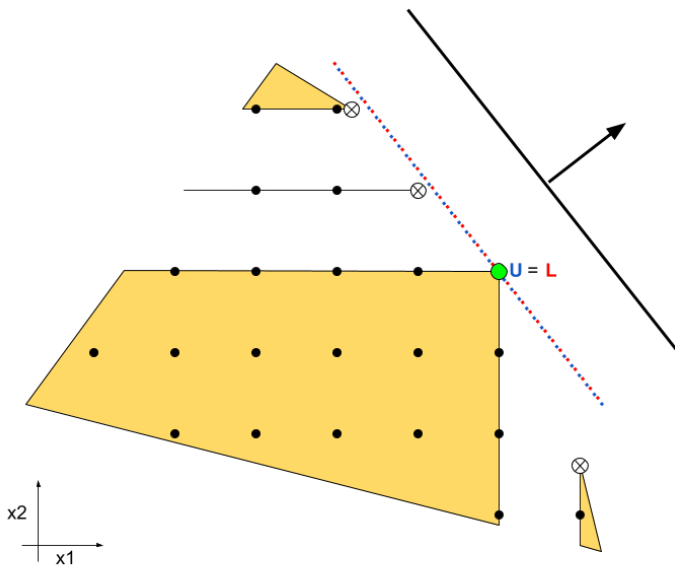
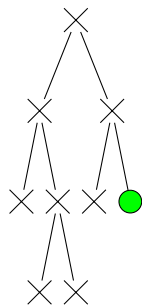
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Branch-and-Bound

Branch: Split the LP recursively over a non-integral variable, i.e.

$$\exists i \leq p \mid x_i^* \notin \mathbb{Z}$$

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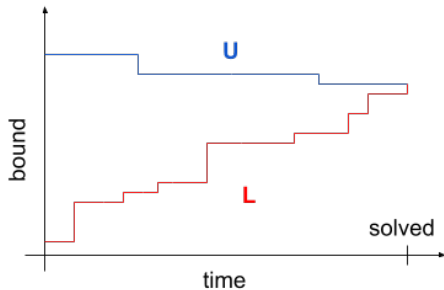
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Note: A time limit is used to ensure termination.

Branch-and-bound: a sequential process

Sequential decisions:

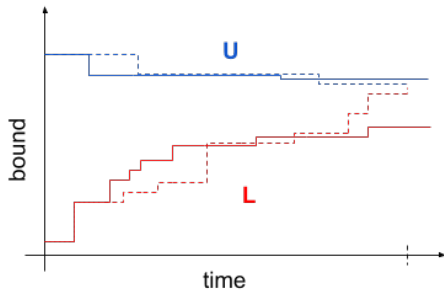
- ▶ variable selection (branching)
- ▶ node selection
- ▶ *cutting plane selection*
- ▶ *primal heuristic selection*
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- ▶ ...



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Branching Policy

It is also called as **variable selection policy**.

Policy Objective: Given a B&B node i.e. MILP, select a variable $i \leq p \mid x_i^* \notin \mathbb{Z}$ so that the final size of the tree is minimum (a proxy for running time).

A gold standard: Strong Branching (impractical)

Strong branching¹: one-step forward looking (greedy)

- ▶ solve both LPs **for each candidate variable**
- ▶ select the variable resulting in tightest relaxation
- + small trees
- computationally expensive

¹D. Applegate et al. (1995). Finding cuts in the TSP. [Tech. rep. DIMACS](#); J. Linderoth et al. (May 1999). A Computational Study of Search Strategies for Mixed Integer Programming.

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$$i_{SB}^* = \arg \max_i \text{score}_{SB,i}$$

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Learning to branch

Objective:

Given a distribution of problem sets, find a branching policy that yields a shortest tree on an average.

Exploits statistical correlation across problem sets.

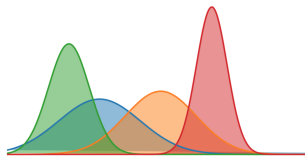


Figure: Application specific distribution

Learning to branch

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Well studied problem (not an exhaustive list)

- ▶ Gasse et al., 2019 \implies offline imitation learning using GCNN
- ▶ Nair et al., 2020 \implies uses GCNNs to design other heuristics
- ▶ Chen et al., 2022 \implies studies the limitations of existing GNNs to represent MILPs

Learning to branch: GNNs

Gasse et al., 2019 uses Graph Neural Networks to imitate the strong branching policy *through classification framework*

- + superior representation power
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Model inputs

Inputs to the GNN is a **bipartite-representation of MILP**: G

GNNs: Bipartite Representation of MILPs

Natural representation : variable / constraint bipartite graph

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v_0

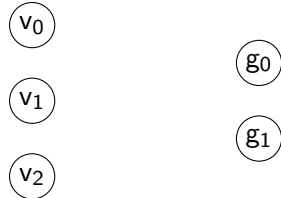
v_1

v_2

- v_i : variable features (type, coef., bounds, LP solution...)

GNNs: Bipartite Representation of MILPs

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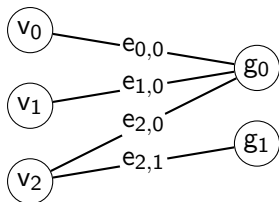
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- ? Can we further improve the performance? (Gupta, Khalil, et al., 2022)

Hybrid Models for Learning to Branch (NeurIPS 2020)

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Model Architecture

Training Protocols

Lookback for Learning to Branch
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MILP Solvers



MILP solvers do not use GPUs.

Use of GNNs can get infeasible in the following scenarios

- ▶ No GPUs: It will be infeasible to incorporate GNNs as a branching policy in any of the available solvers
- ▶ Parallel MILP solving: As a single GPU can only fit a limited number of GNNs, when several 100s of MILPs need to be solved in parallel, GNNs can get infeasible

Runtime performance

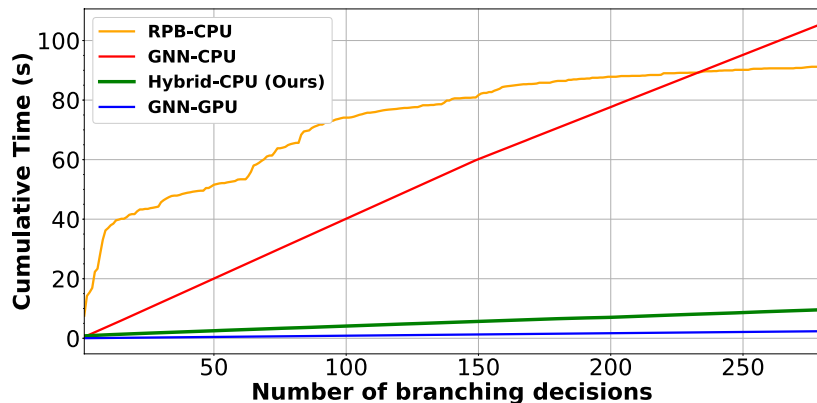


Figure: Cumulative time cost of different branching policies: (i) the default internal rule RPB of the SCIP solver; (ii) a GNN model (using a GPU or a CPU); and (iii) our hybrid model. Clearly the GNN model requires a GPU for being competitive, while our hybrid model does not. (Measured on a capacitated facility location problem, medium size).

Data Extraction

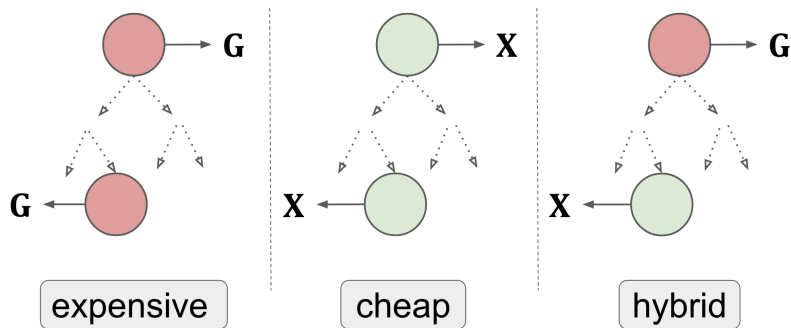


Figure: Data extraction strategies: bipartite graph representation G at every node (expensive); candidate variable features X at every node (cheap); bipartite graph at the root node and variable features at tree node (hybrid).

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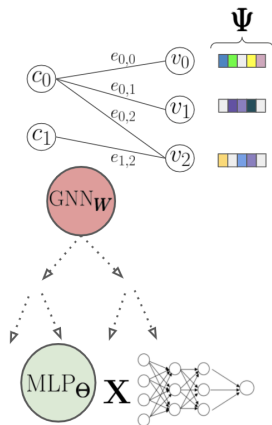
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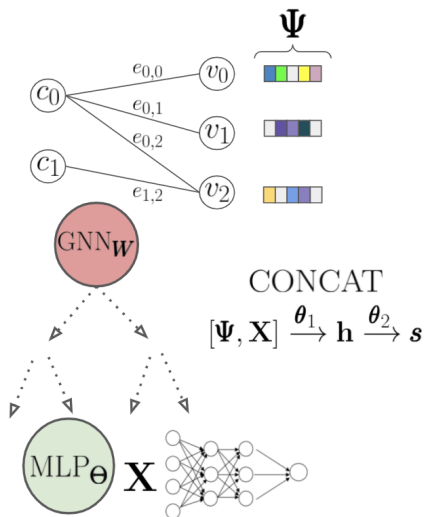
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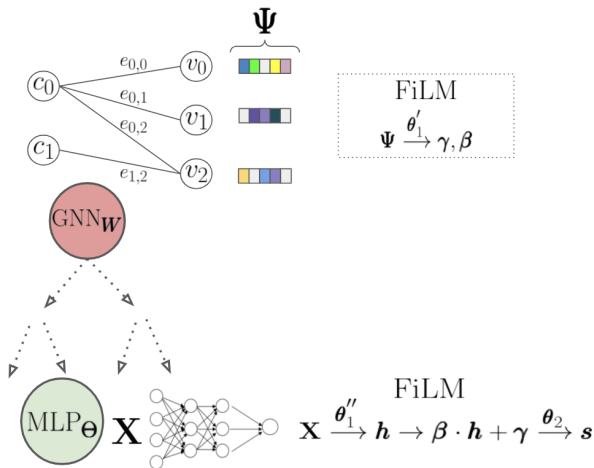
Model Architecture



Model Architecture: CONCAT

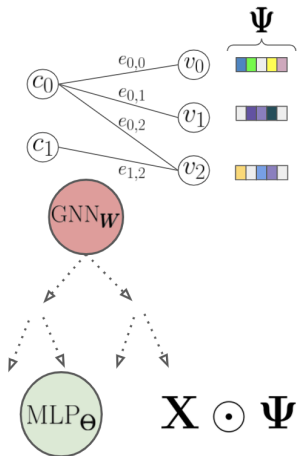


Model Architecture: FiLM



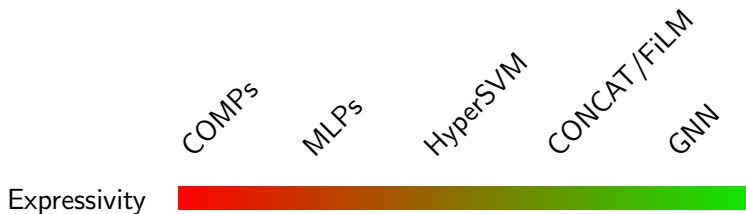
Perez et al., 2018 first proposed FiLM for visual question answering task

Model Architecture: HyperSVM

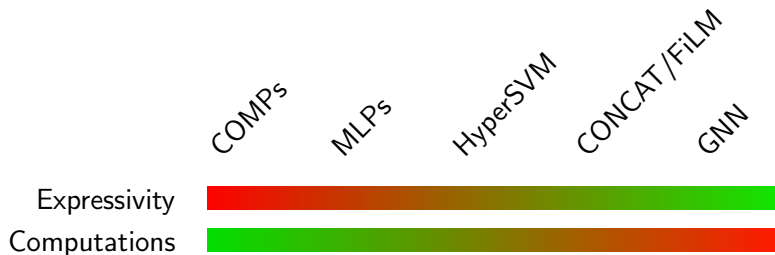


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Model Architecture



Model Architecture



Model Architecture: Performance

End-to-end training

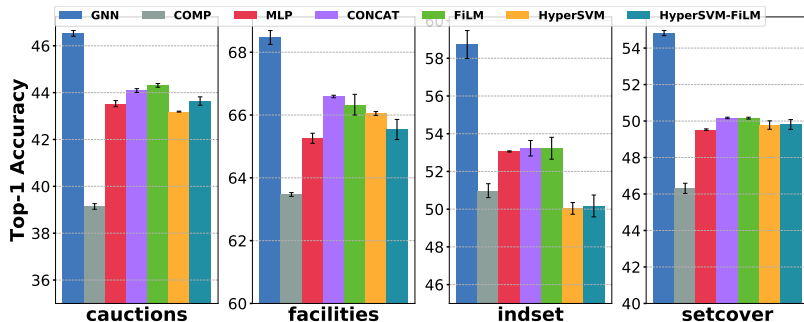


Figure: Test accuracy of the different models, with a simple e2e training protocol.

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Training Protocols

To enhance the generalization power of the learned models on the bigger instances

Training Protocols: Loss weights

A good decision closer to the root node is more important than the ones far away from it.

Table: Effect of different sample weighting schemes on combinatorial auctions (big) instances, with a simple MLP model. $z \in [0, 1]$ is the ratio of the depth of the node and the maximum depth observed in a tree.

Type	Weighting scheme	Nodes	Wins
Constant	1	9678	10/60
Exponential decay	$e^{-0.5z}$	9793	10/60
Linear	$(e^{-0.5} - 1) * z + 1$	9789	12/60
Quadratic decay	$(e^{-0.5} - 1) * z^2 + 1$	9561	14/60
Sigmoidal	$(1 + e^{-0.5}) / (1 + e^{z-0.5})$	9534	14/60

Training Protocols: Knowledge Distillation

Knowledge distillation (KD):² Use the output of an expert GNN from [Gasse et al., 2019](#) as a target for the model.

KD reweights the samples so that the student doesn't attempt to sharply classify samples that even the teacher didn't succeed with (i.e. the logits have higher entropy for the more difficult samples) [Phuong et al., 2019](#).

Table: Test accuracy of FiLM, using different training protocols.

	cautions	facilities	indset	setcover
Pretrained GNN	44.12 \pm 0.09	65.78 \pm 0.06	53.16 \pm 0.51	50.00 \pm 0.09
e2e	44.31 \pm 0.08	66.33 \pm 0.33	53.23 \pm 0.58	50.16 \pm 0.05
e2e & KD	44.10 \pm 0.09	66.60 \pm 0.21	53.08 \pm 0.3	50.31 \pm 0.19

²[G. Hinton et al. \(2015\)](#). Distilling the knowledge in a neural network.

Training Protocols: Auxiliary Task

Auxiliary Task (AT): No additional data required. We force the variable representations to be far apart from each other.

- ▶ ED : Maximum distance between these representations in euclidean space
- ▶ MHE³ : Uniform distribution of these representations over a unit hypersphere

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e2e & KD	44.10 \pm 0.09	66.60 \pm 0.21	53.08 \pm 0.3	50.31 \pm 0.19
e2e & KD & AT	44.56 \pm 0.13	66.85 \pm 0.28	53.68 \pm 0.23	50.37 \pm 0.03

³W. Liu et al. (2018). Learning towards minimum hyperspherical energy.

B&B Performance (Runtime)

Finally, the learned models are used as a branching policy in SCIP solver⁴.

Hybrid models have a better runtime performance on average than other baselines as evaluated on CPU only machines.

Model	Time	Easy			Time	Medium			Time	Hard		
		Wins	Nodes			Wins	Nodes			Wins	Nodes	
FSB	42.5	1 / 60	13		313.3	0 / 59	75		997.2	0 / 51	50	
PB	31.4	4 / 60	139		177.7	4 / 60	384		712.6	3 / 56	309	
RPB	36.9	1 / 60	23		214.0	1 / 60	152		794.8	2 / 54	99	
COMP	30.4	3 / 60	120		172.5	4 / 60	347		633.4	6 / 57	294	
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B&B Performance (Runtime)

Model	Time	Small		Nodes	Time	Medium		Nodes	Time	Big		Nodes
		Wins				Wins				Wins		
FSB	42.53	1 / 60		13	313.33	0 / 59		75	997.23	0 / 51		50
PB	31.35	4 / 60		139	177.69	4 / 60		384	712.45	3 / 56		309
RPB	36.86	1 / 60		23	213.99	1 / 60		152	794.80	2 / 54		99
COMP	30.37	3 / 60		120	172.51	4 / 60		347	633.42	6 / 57		294
GNN	39.18	0 / 60		112	209.84	0 / 60		314	748.85	0 / 54		286
FiLM (ours)	24.67	51 / 60		109	136.42	51 / 60		325	531.70	46 / 57		295
GNN-GPU	28.91	- / 60		112	150.11	- / 60		314	628.12	- / 56		286
Capacitated Facility Location												
FSB	27.16	0 / 60		17	582.18	0 / 45		116	2700.00	0 / 0		n/a
PB	10.19	0 / 60		286	94.12	0 / 60		2451	2208.57	0 / 23		82 624
RPB	14.05	0 / 60		54	94.65	0 / 60		1129	1887.70	7 / 27		48 395
COMP	9.83	3 / 60		178	89.24	0 / 60		1474	2166.44	0 / 21		52 326
GNN	17.61	0 / 60		136	242.15	0 / 60		1013	2700.17	0 / 0		n/a
FiLM (ours)	8.73	57 / 60		147	63.75	60 / 60		1131	1843.24	20 / 26		37 777
GNN-GPU	8.26	- / 60		136	53.56	- / 60		1013	1535.80	- / 36		31 662
Set Covering												
FSB	6.12	0 / 60		6	132.38	0 / 60		71	2127.35	0 / 28		318
PB	2.76	1 / 60		234	25.83	0 / 60		2765	393.60	0 / 59		13 719
RPB	4.01	0 / 60		11	26.36	0 / 60		714	210.95	29 / 60		4701
COMP	2.76	0 / 60		82	29.76	0 / 60		930	494.59	0 / 54		5613
GNN	2.73	1 / 60		71	22.26	0 / 60		688	257.99	6 / 60		3755
FiLM (ours)	2.13	58 / 60		73	15.71	60 / 60		686	217.02	25 / 60		4315
GNN-GPU	1.96	- / 60		71	11.70	- / 60		688	121.18	- / 60		3755
Combinatorial Auctions												
FSB	673.43	0 / 53		47	1689.75	0 / 20		10	2700.00	0 / 0		n/a
PB	172.03	2 / 57		5728	753.95	0 / 45		1570	2685.23	0 / 1		38 215
RPB	59.87	5 / 60		603	173.17	11 / 60		205	1946.51	9 / 21		2461
COMP	82.22	1 / 58		847	383.97	1 / 52		267	2393.75	0 / 6		5589
GNN*	44.07	15 / 60		331	625.23	1 / 50		599	2330.95	0 / 10		687
FiLM* (ours)	52.96	37 / 55		376	131.45	47 / 54		264	1823.29	12 / 15		1201
GNN-GPU*	31.71	- / 60		331	63.96	- / 60		599	1158.59	- / 27		685
Maximum Independent Set												

B&B Performance (Optimality Gap)

Hybrid models also have the least optimality gap at the end of the time limit as compared to other baselines as evaluated on CPU only machines.

Table: Mean optimality gap (lower the better) of commonly unsolved "big" instances (number of such instances in brackets).

	setcover (33)	indset (39)
FSB	0.1709	0.0755
PB	0.0713	0.0298
RPB	0.0628	0.0252
COMP	0.0740	0.0252
GNN	0.1039	0.0341
FiLM	0.0597	0.0187

Runtime performance

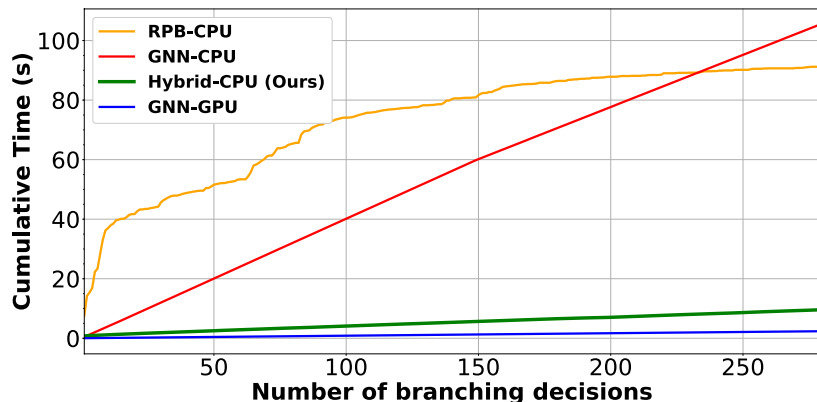


Figure: Cumulative time cost of different branching policies: (i) the default internal rule RPB of the SCIP solver; (ii) a GNN model (using a GPU or a CPU); and (iii) our hybrid model. Clearly the GNN model requires a GPU for being competitive, while our hybrid model does not. (Measured on a capacitated facility location problem, medium size).

Open questions

- ▶ scaling to the real-world problems
- ▶ reinforcement learning: still a lot of challenges
- ▶ interpretation: which variables are chosen? Why ?
- ▶ learning in collaboration with other heuristics, e.g, cut selection, node selection, etc.
- ▶ meta-learning to transfer to unseen instances



Paper: <https://arxiv.org/abs/2006.15212>



Code: <https://github.com/pg2455/Hybrid-learn2branch>



Peer-reviews:
<http://bit.ly/3XU9E8W>

QR Codes generated via <https://www.qr-code-generator.com/>

Lookback for Learning to Branch (TMLR 2022)

Outline

Problem formulation

Hybrid Models for Learning to Branch
(NeurIPS 2020)

Lookback for Learning to Branch
(TMLR 2022)

- Lookback condition

- Loss target

- Regularizer

- Evaluation

- Conclusion

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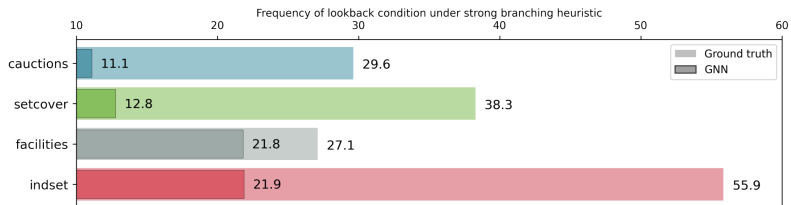
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Lookback condition in strong branching

Strong branching heuristic exhibits the following condition:
Parent's second best choice is *often* the child's best choice.

Frequency of Lookback condition



Frequency of Lookback condition

Instances	Description	number of parent-child pairs collected	number of parent-child pairs exhibiting the lookback property	Frequency of the lookback property
CORLAT	Corridor planning in wildlife management	5082	1765	34.73%
RCW	Red-cockaded woodpecker diffusion conservation	5115	1952	38.16%

Frequency of the lookback property in the real-world instances is as prevalent as in the synthetic instances considered in the main paper. These instances are made available by [Dilkina et al., 2017](#).

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Loss targets

We consider two types of targets

(\mathcal{Z} is the set of all the second best branching variables)

Original one-hot encoded target,

y

$$y_i = \begin{cases} 1, & i = i_{SB}^* \\ 0, & \text{otherwise} \end{cases}$$

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$$\theta_y^* = \arg \min_{\theta} \frac{1}{N} \sum_{k=1}^N CE(f_{\theta}(\mathcal{G}_k), y_k)$$

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Second-best ϵ -smoothed target,
 z

$$z_i = \begin{cases} 1 - \epsilon, & i = i_{SB}^* \\ \frac{\epsilon}{|\mathcal{Z}|}, & i \in \mathcal{Z} \\ 0, & \text{otherwise} \end{cases}$$

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(NeurIPS 2020)

Lookback for Learning to Branch
(TMLR 2022)

Lookback condition

Loss target

Regularizer

Evaluation

Conclusion

Parent-As-Target (PAT) regularizer

We consider a regularizer to encourage the lookback property in GNNs

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$$\text{loss}_{PAT} = 1\{\text{Lookback}_i\} \cdot CE(f_\theta(\mathcal{G}_i), f_\theta(\mathcal{G}_i^{\text{parent}})[\mathcal{C}_i]),$$

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Performance evaluation

We will consider three different set of parameters

- ▶ Choice of the target:
 - ▶ One-hot encoded, y
 - ▶ Second-best ϵ -smoothed, z
- ▶ Strength of the PAT regularizer, $\lambda_{PAT} \in \{0, 0.01, 0.1, 0.2, 0.3\}$
- ▶ Strength of the l_2 -regularizer, $\lambda_{l_2} \in \{0.0, 0.01, 0.1, 1.0\}$

Performance evaluation

$$\theta_y = \arg \min_{\theta, \lambda_{l_2}} \frac{1}{N} \sum_{k=1}^N CE(f_{\theta}(\mathcal{G}_k), y_k) + \lambda_{l_2} \cdot \|\theta\|_2$$

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$$\theta_{PAT} = \arg \min_{\theta, v, \lambda_{l2}, \lambda_{PAT}} \frac{1}{N} \sum_{k=1}^N CE(f_{\theta}(\mathcal{G}_k), v) + \lambda_{l2} \cdot \|\theta\|_2 + \lambda_{PAT} \cdot \text{loss}_{PAT}$$

Performance evaluation: Instances

- ▶ **Small** instances are used to collect training data of parent-child nodes by solving these instances using the strong branching heuristic as the variable selection policy in the solver

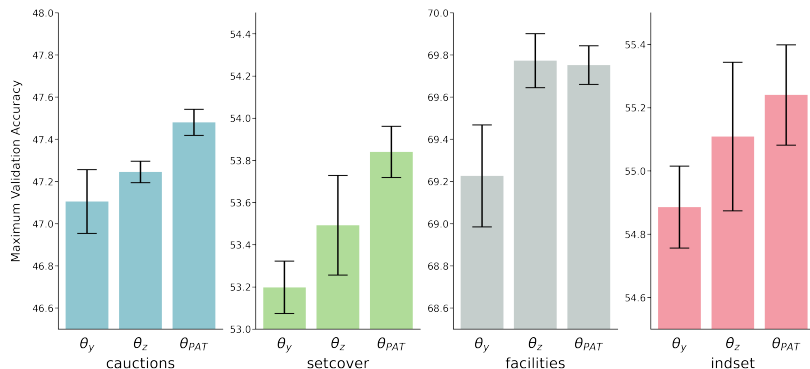
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- ▶ **Big** instances are used to report performance evaluation

Model selection criterion: Validation accuracy



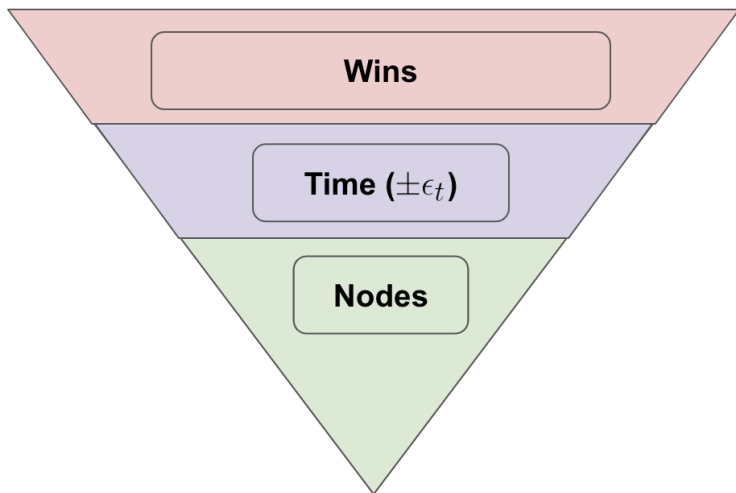
Top-1 accuracy (1-standard deviation) on validation dataset.

Model selection criterion: Out-of-distribution performance

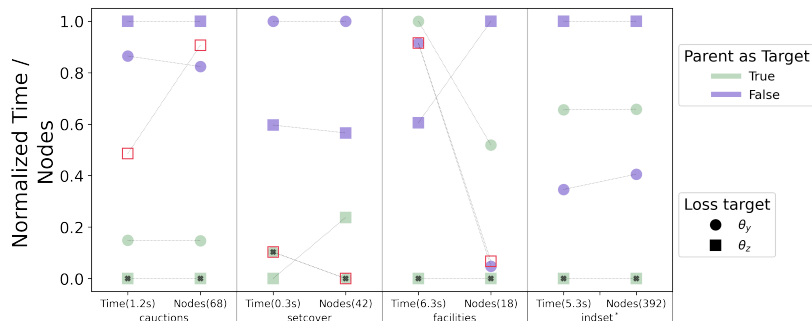
We solve 100 **medium** instances and collect the following metrics

- ▶ Wins: Number of times a model solved the instance fastest
- ▶ Time: 1-shifted geometric mean of time taken to solve each instance
- ▶ Nodes: 1-shifted geometric mean of nodes taken in the B&B tree of the *commonly solved instances*

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We plot the range-normalized (range is specified in parenthesis) Time and Node performance of the selected models. The centered "X" black mark shows the final models that were selected to be used for evaluating the performance on Big instances. The points with a red outline show the performance of the models selected according to the best validation accuracy (Note that we omit such models for indset as it distorts the scale of the plot.)

Final performance

Model	Time	Time (c)	Wins	Solved	Nodes (c)
FSB*	n/a	n/a	n/a	n/a	n/a
RPB	626.81	434.92	1	80	17 979
TUNEDRPB	644.20	450.06	0	80	18 104
GNN	507.06	333.59	14	80	17 145
GNN-PAT (ours)	477.26	310.22	69	84	16 388

Combinatorial Auction (Bigger)

Figure: Evaluation metrics on Big instances with a time budget of 30 minutes per instance

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Optimality gap on commonly unsolved instances

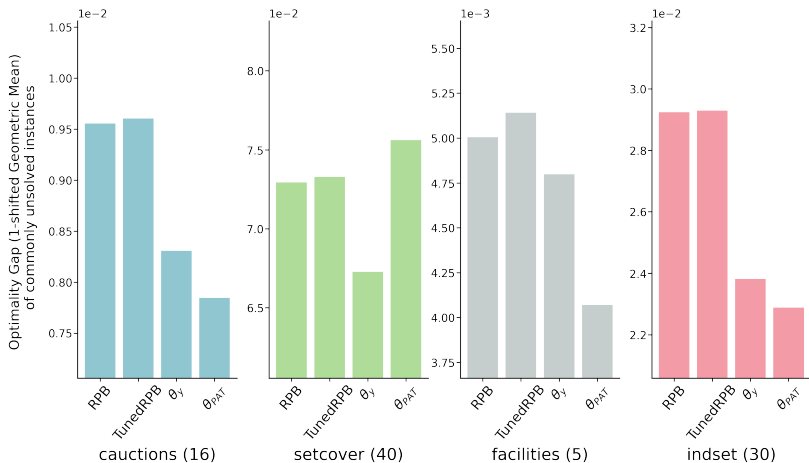


Figure: Mean optimality gap of the *commonly unsolved instances*

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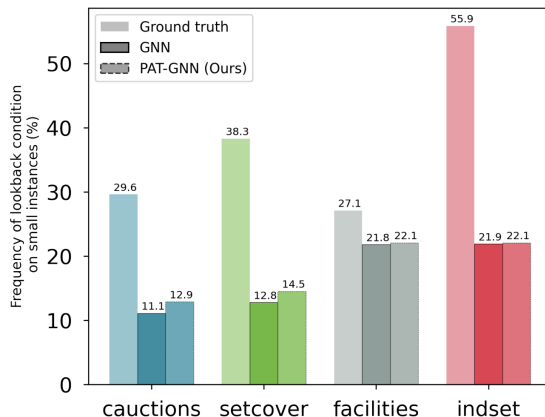
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- ▶ We **proposed** a model selection scheme to incorporate final utility of these models in the objective function
- ▶ Our proposed models outperform the SOTA results

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Paper: <https://arxiv.org/abs/2006.15212>



Peer-reviews:
<https://openreview.net/forum?id=EqpGkw5rvL>

Learning to Branch

Thank you!

Prateek Gupta*, Elias B. Khalil, Didier Chételat, Maxime Gasse,
M. Pawan Kumar, Andrea Lodi, Yoshua Bengio





Slides: www.pgupta.info/talks